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NEWS 4 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update frequency

NEWS 5 Feb 19 Access via Tymnet and SprintNet Eliminated Effective 3/31/02

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NEWS 7 Mar 22 TOXLIT no longer available

NEWS 8 Mar 22 TRCTHERMO no longer available NEWS 9 Mar 28 US Provisional Priorities searched with P in CA/CAplus

and USPATFULL NEWS 10 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY

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NEWS 14 Apr 09 ZDB will be removed from STN
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CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),

AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002

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Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 09747195.str

L1 STRUCTURE UPLOADED

=> d ll L1 HAS NO ANSWERS L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam SAMPLE SEARCH INITIATED 16:07:49 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2725 TO ITERATE

36.7% PROCESSED 1000 ITERATIONS (1 INCOMPLETE) 50 ANSWERS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 51371 TO 57629

PROJECTED ANSWERS: 4311 TO 6261

L2 50 SEA SSS SAM L1

=> d scan 12

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,7-Naphthalenedisulfonic acid, 5-[[4-[[4-(cyanoamino)-6-[(3-sulfophenyl)amino]-1,3,5-triazin-2-yl]amino]benzoyl]amino]-4-hydroxy-3-[[1-sulfo-6-[[2-(sulfooxy)ethyl]sulfonyl]-2-naphthalenyl]azo]- (9CI)
MF C39 H30 N10 O20 S6

PAGE 1-A

PAGE 1-B

- oso₃H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):49

- L2
- 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS [2,2'-Binaphthalene]-1,3',5,6'-tetrasulfonic acid, 8'-[[4-[[3-[[[2-IN (ethenylsulfonyl)ethyl]amino]carbonyl]phenyl]amino]-6-fluoro-1,3,5-triazin-

2-yl]amino]-1'-hydroxy-, tetrasodium salt (9CI) MF $\,$ C34 H27 F N6 O16 S5 . 4 Na

•4 Na

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- MF C40 H42 N14 O10 S2 . 2 Na

PAGE 1-A

O MeO-CH₂-CH₂-NH SO₃H SO₃H
$$\frac{1}{N}$$
 $\frac{1}{N}$ $\frac{1}{N}$

•2 Na

PAGE 1-B

$$\begin{array}{c|c} \text{NH-CH}_2\text{-CH}_2\text{-OMe} & \text{O} \\ \hline \\ \text{N} & \text{NH-CH}_2\text{-CH}_2\text{-OMe} \\ \hline \\ \text{N} & \text{NH-CH}_2\text{-OMe} \\ \end{array}$$

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzaldehyde, 3-nitro-, [4-[(4-nitrophenyl)amino]-6-[2,2,2-trifluoro-1-

09/891,750

(trifluoromethyl)ethoxy]-1,3,5-triazin-2-yl]hydrazone (9CI)
MF C19 H12 F6 N8 O5

$$_{\text{F}_3\text{C}-\text{CH}-\text{O}}^{\text{CF}_3}$$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$
 $_{\text{N}}^{\text{N}}$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C21 H29 F3 N8 O2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzoic acid, 2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-6-[[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]oxy]- (9CI)

MF C19 H20 N6 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 4-[[4-chloro-6-[[4-(2-hydroxy-4-methoxy-5sulfobenzoyl)phenyl]amino]-1,3,5-triazin-2-yl]amino]-2-hydroxy-,
monosodium salt (9CI)

MF C24 H18 Cl N5 O9 S . Na

● Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[[4-[(4acetylphenyl)amino]-6-propoxy-1,3,5-triazin-2-yl]amino]-, disodium salt
(9CI)

MF C42 H42 N10 O10 S2 . 2 Na

•2 Na

PAGE 1-B

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 2,2'-[[6-[(2-hydroxyethyl)amino]-1,3,5-triazine-2,4diyl]bis[imino(6,13-dichloro-4,11-disulfo-10,3triphenodioxazinediyl)imino[6-[(2-hydroxyethyl)amino]-1,3,5-triazine-4,2diyl]imino]]bis- (9CI)

MF C65 H46 C14 N22 O23 S4

PAGE 1-A

PAGE 1-B

- **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzaldehyde, 2-hydroxy-3,5-dinitro-, [4-[(3,4-dimethylphenyl)amino]-6-[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]hydrazone (9CI)
- MF C24 H20 N10 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS ITERATION INCOMPLETE
- IN 1,3,5-Triazin-2-amine, N-[4-(chlorodifluoromethoxy)phenyl]-4,6-diphenoxy(9CI)
- MF C22 H15 C1 F2 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzoic acid, 2-[[4-(cyanoamino)-6-[[8-hydroxy-3,6-disulfo-7-[[4-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]-1-naphthalenyl]amino]-1,3,5-triazin-2-yl]amino]- (9CI)
- MF C29 H23 N9 O15 S4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- MF C43 H43 N11 010 S . 3 H3 N

●3 NH3

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzamide, 2-[[4-[(4-bromophenyl)amino]-6-[[[(3methylphenyl)amino]thioxomethyl]amino]-1,3,5-triazin-2-yl]oxy]- (9CI)
- MF C24 H20 Br N7 O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzaldehyde, 3,5-bis[(4,6-dimethoxy-1,3,5-triazin-2-yl)oxy]- (9CI)
- MF C17 H16 N6 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzamide, 4-methyl-3-[[4-[methyl(3,3,3-trifluoro-2-methylpropyl)amino]-6-[(3R)-3-pyrrolidinylamino]-1,3,5-triazin-2-yl]amino]- (9CI)
- MF C20 H27 F3 N8 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 4,4'-[[6-[[4-[[2-[4-(1,1-dimethylethyl)phenoxy]ethoxy]carbon
yl]phenyl]amino]-1,3,5-triazine-2,4-diyl]diimino]bis-, dimethyl ester
(9CI)

MF C38 H38 N6 O7

PAGE 1-B

__Bu−t

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1,3,5-Triazine, 2,4-dimethoxy-6-(3-nitrophenoxy)- (9CI)

09/891,750

MF C11 H10 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 2-Naphthalenesulfonic acid, 6-amino-5-[[4-[[4-chloro-6-[[3-[[[2-[[2(sulfooxy)ethyl]sulfonyl]ethyl]amino]carbonyl]phenyl]amino]-1,3,5-triazin2-yl]amino]phenyl]azo]-4-hydroxy- (9CI)
- MF C30 H28 C1 N9 O11 S3

C1 N NH C-NH-CH₂-CH₂-S-CH₂-CH₂-OSO₃H

N NH
N OH
$$H_2N$$
SO₃H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzoic acid, 4,4',4''-(1,3,5-triazine-2,4,6-triyltriimino)tris-, tris[3-(pentamethyldisiloxanyl)propyl] ester (9CI)
- MF C48 H78 N6 O9 Si6

PAGE 1-A

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Furancarboxaldehyde, 5-(2,4-dichlorophenyl)-, [4-[(3,4-dimethylphenyl)amino]-6-[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]hydrazone (9CI)

MF C28 H22 C12 N8 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzamide, 3-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]-4-methyl-N-(2-phenylethyl)- (9CI)
- MF C19 H17 C12 N5 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzoic acid, 4-[[4-[(4-methylphenyl)amino]-6-[[5-(phenylamino)-1,3,4-thiadiazol-2-yl]thio]-1,3,5-triazin-2-yl]amino]- (9CI)
- MF C25 H20 N8 O2 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2002 ACS T.2 50 ANSWERS

Benzenesulfonic acid, 4-[[4-[[4-chloro-6-[[4-[[2-ΙN (sulfooxy)ethyl]sulfonyl]phenyl]amino]-1,3,5-triazin-2yl]amino]benzoyl]amino]-, disodium salt (9CI) C24 H21 Cl N6 O10 S3 . 2 Na

MF

●2 Na

PAGE 1-B

__ SO3H

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Benzamide, 2-[[4-[[(1-naphthalenylamino)thioxomethyl]amino]-6-[(4-phenyl-2-IN thiazolyl)amino]-1,3,5-triazin-2-yl]oxy]- (9CI)

C30 H22 N8 O2 S2 MF

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1,7-Naphthalenedisulfonic acid, 4,4'-[2,4,8,10-tetraoxaspiro[5.5]undecane3,9-diylbis[methyleneimino[6-(4-nitrophenoxy)-1,3,5-triazine-4,2diyl]imino]]bis[5-hydroxy-6-[[3-[(2-hydroxyethyl)sulfonyl]phenyl]azo]-,
tetrasodium salt (9CI)

MF C63 H56 N16 O30 S6 . 4 Na

PAGE 1-B

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 3-[[4-[(2,2-dimethylpropyl)methylamino]-6-[[(3S)-1-phenyl-3-pyrrolidinyl]amino]-1,3,5-triazin-2-yl]amino]-4-methyl- (9CI)

MF C27 H36 N8 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Naphthalenedisulfonic acid, 5-[[4-[[4-fluoro-6-[[3-sulfo-4-[3-[[2-(sulfooxy)ethyl]sulfonyl]propoxy]phenyl]amino]-1,3,5-triazin-2-yl]amino]benzoyl]amino]-4-hydroxy-3-[(2-sulfophenyl)azo]- (9CI)

MF C37 H33 F N8 O21 S6

PAGE 1-A

HO3SO-CH2-CH2-S-(CH2)3-0

SO3H

NH

OH

HO3S

NH

HO3S

SO3H

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 2,7-Naphthalenedisulfonic acid, 5-[[4-[[4-[(cyanoamino)carbonyl]-3methylphenyl]amino]-6-fluoro-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[(1sulfo-2-naphthalenyl)azo]- (9CI)
- MF C32 H22 F N9 O11 S3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C31 H27 C1 N8 O9 S3

PAGE 1-B

$$- cH_2 - cH_2 - s - cH = cH_2$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzaldehyde, 4-nitro-, [4-(cyclohexylamino)-6-[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]hydrazone (9CI)

MF C22 H23 N9 O4

$$O_2N$$
 O_2N
 O_2N

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzoic acid, 2-[[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]oxy]-, methyl ester (9CI)
- MF C16 H21 N5 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzamide, 3-[[4-amino-6-[(2,2-dimethylpropyl)methylamino]-1,3,5-triazin-2-yl]amino]-N-methoxy-4-methyl- (9CI)
- MF C18 H27 N7 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C45 H38 F N9 O14 S4

PAGE 1-A

PAGE 1-B

-- CH=- CH $_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzenesulfonic acid, 5-[[4-[(4-acetylphenyl)amino]-6-chloro-1,3,5-triazin-2-yl]amino]-2-[2-(2-sulfophenyl)ethenyl]-, disodium salt (9CI)

MF C25 H20 Cl N5 O7 S2 . 2 Na

2 Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 2-[[4-[[[(2-methylphenyl)amino]thioxomethyl]amino]-6-[(4-phenyl-2-thiazolyl)amino]-1,3,5-triazin-2-yl]oxy]- (9CI)

MF C27 H22 N8 O2 S2

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 3,3'-[[6-[[3-(diethylamino)propyl]amino]-1,3,5-triazine-2,4-diyl]bis[imino(6,13-dichloro-4,11-disulfo-10,3-triphenodioxazinediyl)imino[6-[[3-(diethylamino)propyl]amino]-1,3,5-triazine-4,2-diyl]imino]]bis- (9CI)

MF C80 H79 C14 N25 O20 S4

PAGE 1-A

PAGE 1-B

PAGE 1-C

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 4-methyl-N-(1-methylethyl)-3-[[4-[methyl(2-methylpropyl)amino]-6-[(3R)-3-pyrrolidinylamino]-1,3,5-triazin-2-yl]amino]- (9CI)

MF C23 H36 N8 O

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1,3,5-Triazine-2,4-diamine, 6-(2-benzothiazolylthio)-N,N'-bis(3nitrophenyl)- (9CI)

MF C22 H14 N8 O4 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Naphthalenesulfonic acid, 2-[[6-[[4-chloro-6-[[4-[(cyanoamino)carbonyl]3-methylphenyl]amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3-sulfo-2naphthalenyl]azo]- (9CI)

MF C32 H22 Cl N9 O8 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 3-[[8-[[4-[(3-carboxyphenyl)amino]-6-[(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-, diammonium disodium salt (9CI)

MF C29 H24 N8 O12 S2 . 2 H3 N . 2 Na

● 2 NH3

2 Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Propenal, 2-bromo-3-phenyl-, [4-[(4-nitrophenyl)amino]-6-(phenylamino)1,3,5-triazin-2-yl]hydrazone (9CI)

MF C24 H19 Br N8 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Propenal, 2-methyl-3-phenyl-, [4-[(2-methylphenyl)amino]-6-[(4-nitrophenyl)amino]-1,3,5-triazin-2-yl]hydrazone (9CI)

MF C26 H24 N8 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Naphthalenecarboxylic acid, 2-[4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]benzoyl]hydrazide (9CI)

MF C23 H20 N6 O4

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 4-[[4-chloro-6-[[4-(2-phenylethenyl)-3-sulfophenyl]amino]-1,3,5-triazin-2-yl]amino]-, 1-ethyl ester, monosodium salt (9CI)

MF C26 H22 Cl N5 O5 S . Na

Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 2,2'-[1,3-phenylenebis[iminocarbonylimino(6-sulfo-3,1phenylene)azo(8-sulfo-4,1-naphthalenediyl)imino(6-fluoro-1,3,5-triazine4,2-diyl)imino]]bis- (9CI)

MF C60 H42 F2 N18 O18 S4

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 3,3'-[[6-[[3-(diethylamino)propyl]amino]-1,3,5-triazine-2,4diyl]bis[imino(6,13-dichloro-4,11-disulfo-10,3triphenodioxazinediyl)imino[6-[methyl(2-sulfoethyl)amino]-1,3,5-triazine4,2-diyl]imino]]bis- (9CI)

MF C72 H61 C14 N23 O26 S6

PAGE 1-B

PAGE 1-C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzoic acid, 3-[[4-[(4-carboxyphenyl)amino]-6-[(4-chlorophenyl)thio]1,3,5-triazin-2-yl]amino]- (9CI)

MF C23 H16 C1 N5 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 2-[[4-[(4-bromophenyl)amino]-6-[[[(3nitrophenyl)amino]carbonyl]amino]-1,3,5-triazin-2-yl]oxy]- (9CI)

MF C23 H17 Br N8 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

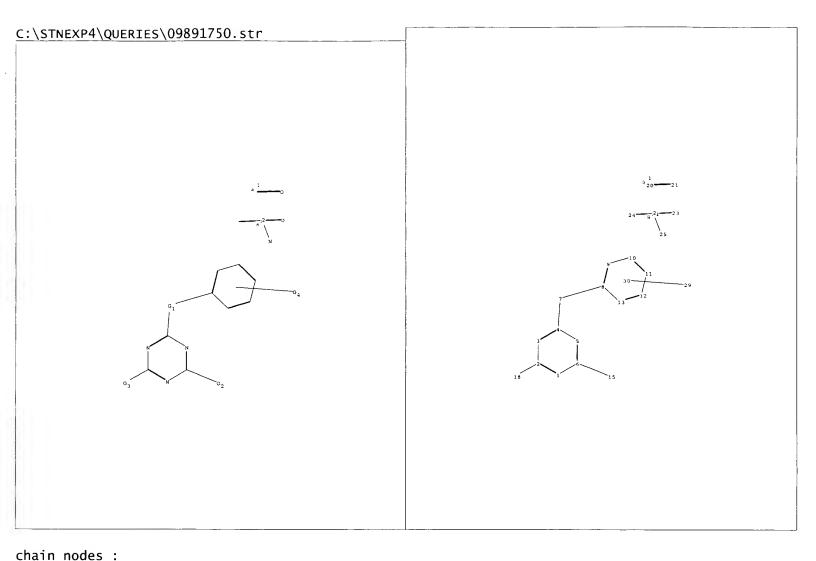
ALL ANSWERS HAVE BEEN SCANNED

=> log y
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.76 0.97

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 15:CLASS 18:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 29:CLASS 30:CLASS

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7 15 18 20 21 22 23 24 25 29
ring nodes:
    1 2 3 4 5 6 8 9 10 11 12 13
chain bonds:
    2-18 4-7 6-15 7-8 20-21 22-23 22-24 22-25
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13
exact/norm bonds:
    2-18 4-7 6-15 7-8 20-21 22-23 22-24 22-25
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13
isolated ring systems:
    containing 8:

G1:0,S,N,CH
G2:X,O,N
G3:0,S,N,X,Cb,Ak
```

G4:NO2,[*1],[*2]

Match level: